High Production Volume (HPV) Chemical Challenge Program:
Final Revised Test Plan and Assessment with Robust Study Summaries
for
Linear and Branched Alkylbenzene Sulfonic Acids and Derivatives
Part I: Test Plan and Assessment for LAS/ABS Category

Prepared and submitted by

The Soap and Detergent Association (SDA) Linear Alkylbenzene Sulfonate (LAS)/ Alkyl Benzene Sulfonate (ABS) Consortium

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1 Introduction

This data availability summary and test plan is for a group of linear (LAS) and branched (ABS) alkylbenzene sulfonates classified as high production volume (HPV) chemicals according to criteria established by the United States Environmental Protection Agency's (U.S. EPA) HPV Chemical Challenge Program, i.e., >1,000,000 pounds manufactured in or imported into the U.S. annually. Nine chemicals, each described by one or more Chemical Abstract Service Registration Number (CAS RN), are indicated **in bold** in Table 1-1. In total, they are produced/imported into the U.S. at about 21,000,000 pounds on an annual basis. This estimate is based on volumes provided by the consortium members named below from their 2002-2006 reporting data. While there may be other minor producers of these nine sponsored chemicals, it is believed that 21 million pound is representative of the total in the U.S. for the category.

LAS/ABS chemicals are anionic surfactants used to lower the surface tension of water. These chemicals are used in cleaning products for home, institutional, and industrial use. Typical formulated products include car wash liquids, laundry detergents, liquid dish detergents, hard surface cleaners, dry cleaning products, waterless hand cleaners, and industrial cleaners. They are also used in emulsion polymerisation (e.g., some agriculture products), as dye dispersants in the textile industry, in paint strippers, in some specialized personal care products**,** and for "bubble making" solutions in children's products. Based on data provided by the Consortium members, the volume produced or imported in the U.S. is used in the following manner: ~56% is used in industrial/commercial products, ~24% is used as intermediates in chemical manufacturing, and ~20% is used in consumer products. Industrial/commercial products usually contain 60-90% LAS/ABS and consumer products 5-30% LAS/ABS.

Table 1.1 – All CAS RNs included in this LAS-ABS category for purposes of "read-across"

#	CAS RN	Chemical Name
1	**26264-05-1**	**Benzenesulfonic acid, dodecyl-, compd. with 2-propanamine (1:1)**
2	68584-24-7	Benzenesulfonic acid, C10-16-alkyl derivs., compds with 2-propanamine
3	**90218-35-2**	**Benzenesulfonic acid, dodecyl-, branched, compd. with 2-propanamine (1:1)**
4	**27323-41-7**	**Benzenesulfonic acid, dodecyl-, compd. with 2,2',2''-nitrilotris[ethanol](1:1)**
5	68411-31-4	Benzenesulfonic acid, C10-13-alkyl derivs., compds. with Triethanolamine
6	70528-84-6	Benzenesulfonic acid, dodecyl, branched, compds. with Triethanolamine
7	**26264-06-2**	**Benzenesulfonic acid, dodecyl-, calcium salt**
8	**68411-32-5**	**Benzenesulfonic acid, dodecyl-, branched**
9	**68608-88-8**	**Benzenesulfonic acid, mono-C11-13-branched alkyl derivs.**
10	**68608-89-9**	**Benzenesulfonic acid, mono-C11-13-branched alkyl derivs., sodium salts**
11	**68953-96-8**	**Benzenesulfonic acid, mono-C11-13-branched alkyl derivs., calcium salts**
12	**70528-83-5**	**Benzenesulfonic acid, dodecyl-, branched, calcium salts**
13	42615-29-2	Benzenesulfonic acid, alkyl deriv., linear
14	68584-26-9	Benzenesulfonic acid, C10-16-alkyl derivs., magnesium salts
15	27176-87-0	Benezenesulfonic acid, dodecyl-
16	68411-30-3	Benzenesulfonic acid, C10-13 alkyl derivs., sodium salt

Notes: 1) **In bold, CAS RNs sponsored by this Consortium under the EPA HPV Chemical Challenge program or Extended HPV (eHPV) initiative**

2) "dodecyl" indicates C12, a twelve carbon chain

Nine CAS RNs (**bolded** in Table 1.1) are sponsored by The Soap and Detergent Association (SDA) LAS/ABS Consortium. Because of nomenclature modifications adopted to provide more descriptive characterization of the chemical entities, three of the sponsored chemicals are identified by additional chemical names (commercial synonyms) and CAS RNs. These synonymous chemicals are entry #2, #5 and #6; that is, chemical #2 is commercially synonymous with the sponsored chemicals #1 & #3, and chemicals #5 and #6 are commercially synonymous with the sponsored chemical #4. Both the "old" chemical names and CAS RN and the "new" chemical names and CAS RNs currently are in use and describe the same chemical entities in commerce before and after the 2002 IUR listing. Specifically, it should be noted that:

- The commercial substance benzenesulphonic acid, dodecyl-, compd. with 2-propanamine (sponsored CAS RN 26264-05-1) is also known as benzenesulfonic acid, C10-16-alkyl derivs., compds. with 2-propanamine, linear (synonymous CAS RN 68584-24-7), and as benzenesulfonic acid, dodecyl-, branched, compds. with 2-propanamine, branched (sponsored CAS RN 90218-35-2).
- The commercial substance benzenesulfonic acid, dodecyl-, compd. with 2,2′,2″-nitrilotris[ethanol](1:1) (sponsored CAS RN 27323-41-7) is also known as benzenesulfonic acid, C10-13-alkyl derivs., compds. with triethanolamine, linear (synonymous CAS RN 68411-31-4), and as benzenesulfonic acid, dodecyl, branched, compds. with triethanolamine, branched (synonymous CAS RN 70528-84-6).

Entry #13 and #14 in Table 1.1 (CAS RNs 42615-29-2 and 68584-26-9) are included as supporting chemicals that are structurally very similar to the sponsored chemicals and for which there are extensive toxicological data. Entry #15 and #16 in Table 1.1 CAS RNs 27176-87-0 and 68411-30-3) are two additional supporting chemicals for which there are extensive data from previous OECD or EPA HPV chemical submissions.

The Consortium is comprised of the following companies:

Akzo Nobel Surface Chemistry LLC
Baker Petrolite Corporation
Rhodia Inc.
Stepan Company

The Consortium assembled and reviewed publicly available endpoint data including similar submissions to the OECD and U.S. EPA HPV chemical programs. Also, they collected proprietary data available within their organizations. They developed a summary of the available data and a test plan for the sponsored chemicals[1].

While this summary focuses on available publicly and privately held data for the nine sponsored chemical entities that share close structural and behavioral similarities, there are also SIDS endpoint data for four additional 'supporting chemicals' included in this submission. These additional data are clearly indicated in the document. The sources for these additional data include: (1) the Linear Alkylbenzene Sulfonate (LAS) Category sponsored by the Industry

[1] The consortium provided an interim submission for this category in December 2002. That submission included 6 sponsored chemicals, 3 supporting chemicals, 3 synonymous chemicals, 32 references and 42 robust study summaries. The current (2008) submission includes 9 sponsored chemicals, 4 supporting chemicals, 3 synonomous chemicals, 91 references and 196 robust study summaries.

Coalition for the SIDS Assessment of LAS (in accordance with the International Council of Chemical Associations (ICCA) High Production Volume Chemical Initiative), and (2) the Linear Alkylbenzene (LAB) Sulfonic Acid Category sponsored by the LAB Sulfonic Acid Coalition (in accordance with the U.S. HPV Challenge Program).

2 Data Collection, Review and Summary

The following steps were followed in the preparation of the submission:

1. comprehensive literature search and retrieval of SIDS-endpoint data (and some beyond-SIDS endpoints) for the nine chemicals using complimentary CIS (Chemical Information Systems) and EU (European Union) data sources,
2. search and retrieval by the Consortium member companies of previously unpublished ("in-house") SIDS-endpoint data (and some beyond-SIDS endpoints), along with volume and use information for the nine chemicals,
3. review of all available data and determination of data quality,
4. preparation of robust study summaries for each of the reviewed studies,
5. development and justification of a category to support "read-across" as part of the assessment (this includes the data for the nine sponsored chemicals, data for chemically related substances, and results of structure-activity relationships (SAR) for physical-chemical properties and aquatic toxicity using the ECOSAR model (v0.99h)), and
6. construction of a SIDS data matrix and discussion of data adequacy and/or gaps.

2.1 Public and In-House Records

The literature search employed a strategy utilizing databases available from the U.S. Chemical Information Systems and the European International Uniform Chemical Information Database (IUCLID) and Institute For Systems, Informatics And Safety (ISIS) ECDIN (Environmental Chemicals Data Information Network) databases. These databases include:

- *Registry of Toxic Effects of Chemical Substances (RTECS)*
- *Toxic Substances Control Act Test Submissions (TSCATS)*
- *Integrated Risk Information System (IRIS)*
- *Chemical Carcinogenesis Research Information (CCRIS)*
- *GENETOX*
- *The Environmental Mutagen Information Center (EMIC)*
- *The Environmental Teratology Information Center (ETIC)*
- *The Developmental and Reproductive Toxicology Database (DART)*
- *The Catalogue of Teratogenic Agents (CTA)*
- *ENVIROFATE, DATALOG, AQUIRE, PHYOTOX and TERRATOX*

3 Data Reliability

In accordance with U.S. HPV Challenge Program guidance (i.e., Determining Adequacy of Existing Data), data reliability was established following the rules described by Klimisch et al. (1997). The Klimisch scoring system results are presented in the robust study summaries as "reliability" values. Key features for scoring include: test substance identification; Good Laboratory Practices (GLP) vs. non-GLP studies; details of test methodology; and the

importance of the availability of statistical analyses for establishing the difference between treatment and control groups. The use of sound scientific judgement is acknowledged as an important principle for assessing data adequacy and reliability. The following four categories of reliability are identified in the Klimisch scoring system. Each study/data point included in this assessment is assigned one of these four scores:

1 **Reliable without Restriction**: Includes studies or data complying with GLP procedures, and/or with valid and/or internationally accepted testing guidelines, or in which the key test parameters are documented and comparable to these guidelines.

2 **Reliable with Restrictions:** Includes studies or data in which key test parameters are documented but vary slightly from test guidelines. Also included are citations from published summary reports (e.g., European Commission IUCLID Datasets and other synthesis type documents) where the original study reports were not obtained and independently reviewed by the LAS/ABS Consortium, but the data sources are documented and underwent a previous professional review that concluded the data are reliable.

3 **Not Reliable:** Includes studies or data in which there are interferences, or that use non-relevant organisms or exposure routes, or which were carried out using unacceptable methods, or where documentation is insufficient.

4 **Not Assignable:** Includes studies or data in which insufficient detail is reported to assign a rating, e.g., listed in material safety data sheets, abstracts or secondary literature but which generally are considered reliable sources of information.

4 Chemical Structure and Composition

Linear (designated "LAS") and non-linear or branched (designated "ABS") alkylbenzene sulfonates are anionic surfactants with molecules characterized by a hydrophobic (apolar) and a hydrophilic (polar) group (see Figure 4.1). As a class of chemicals, they are generally mixtures of closely related isomers and homologues. Each molecule contains an aromatic ring sulfonated at the *para* position and attached to either a linear or a branched alkyl chain at any position except the terminal carbons (Valtorta et al., 2000). Chain lengths vary but are predominantly in the range of C10 to C14. Most commercial LAS/ABS products are mixtures but they can be prepared as pure homologues (e.g., a pure C12).

The LAS/ABS chemicals are prepared by sulfonation of linear and non-linear alkylbenzenes. Linear structures of alkylbenzene (sulfonic acid derivatives) are based on the reaction of an alpha olefin (i.e., R-CH=CH_2) with benzene, in the presence of sulphuric acid (SO_3), with or without a catalyst. Sodium hydroxide (NaOH) or some other salt is used to neutralize. Branched alkylbenzene structures (ABS) can also be prepared by several methods. These include the reaction of propylene (CH_3CH:CH_2) oligomers with benzene, or CH_3-$(CH)_{11}$-phenol ring, in the presence of sulphuric acid (SO_3), with or without a catalyst. Sodium hydroxide (NaOH) or some other salt is used to neutralize.

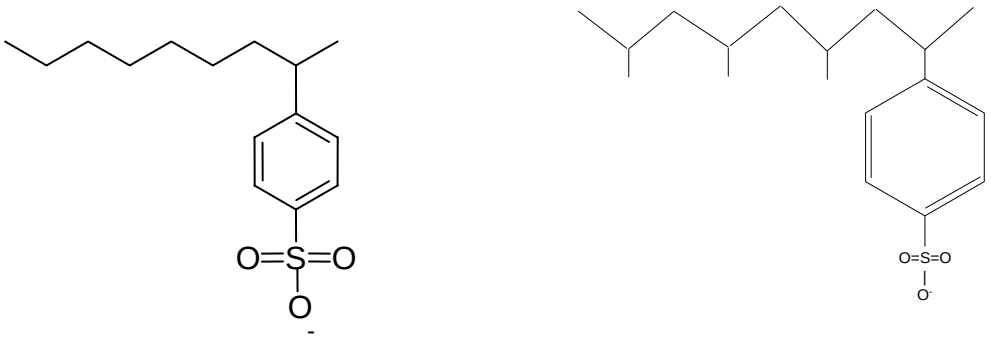
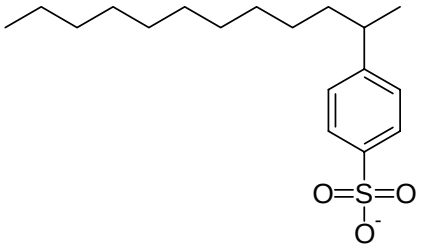
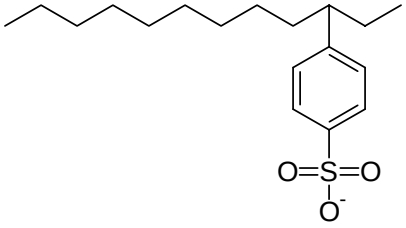


Figure 4-1. Example of structural formula for linear (left) and branched (right) benzene sulfonates.

(a)



(b)



(c)

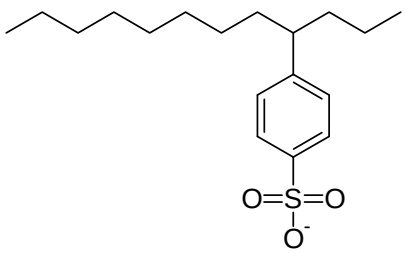


Figure 4-2. General structural formula for (in this case a linear) alkylbenzene sulfonate with the phenyl ring attached to the (a) 2-position, (b) 3-position and (c) 4-position of the alkyl chain.

Using or not using a catalyst, as well as using different catalysts, will produce different amounts of the 2-, 3-, 4-, 5- and 6-phenyl isomers. The 1-phenyl isomer is not formed. Figure 4-2 shows illustrations of general structures of (in this case a linear) alkylbenzene sulfonate (LAS), with the phenyl ring attached to the 2-, 3- or 4-position of the alkyl chain. Table 4-1 presents the typical composition of the product as a function of the catalyst used during synthesis.

Table 4.1 - Typical composition of LAS/ABS structures as a function of catalyst used

Composition	HF catalysed	$AlCl_3$ catalysed	Fixed bed
1-phenyl	0	0	0
2-phenyl	18.5-22.5%	25-33%	25%
3-phenyl	18.5-25.5%	21-24%	21%
4-phenyl	14.5-30%	13-28%	20%
5-phenyl	0-24.5%	0-23%	18%
6-phenyl	0	0-16.5%	14%

4.1 Sponsored Chemicals

The nine CAS RNs sponsored by the Consortium are each depicted below. Each depiction includes the chemical name, the CAS RN, whether the chemical is a linear or branched structure, a representative drawing of the structure itself, and the source of the chemical structure (sources are: online US Library of Medicine – ChemIDplus Advanced or TOXNET, online European Chemical Substances Information System (ESIS), and US EPA ECOSAR v0.99h). It should be noted that, of the several isomeric structures that an LAS/ABS compound can have, only a single phenyl isomer is drawn in the representative structure drawings shown below. Also, the commercial LAS/ABS products are mixtures of various alkyl chain lengths, typically from about C10 to C14. Even the compounds named "dodecyl" (= C12) are, in fact, a mixture of alkyl chain lengths. Table 4-2 shows the typical chain length distribution for the linear LAS/ABS substances. The average carbon number for the alkyl chain for the branched LAS/ABS substances is C12.

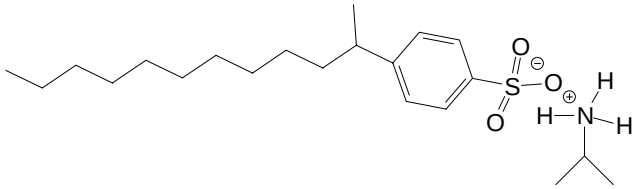
Table 4.2 - Typical chain length distribution of linear LAS/ABS

Chain length	< C10	C10	C11	C12	C13	≥ C14
Amount (%)	≤ 2	≤ 25	~ 40	≥ 25	≤ 15	≤ 2

Where C10 + C11 ≥ 50%; and C10 + C11 + C12 ≥ 85%

Benzenesulfonic acid, dodecyl-, compd. with 2-propanamine (1:1)

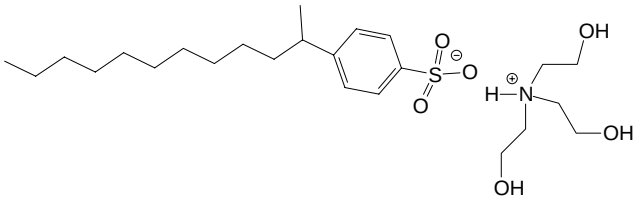
CAS RN: 26264-05-1 (linear)



Source – TOXNET, ECOSAR

Benzenesulfonic acid, dodecyl-, compd. with 2,2′,2″-nitrilotris[ethanol](1:1)

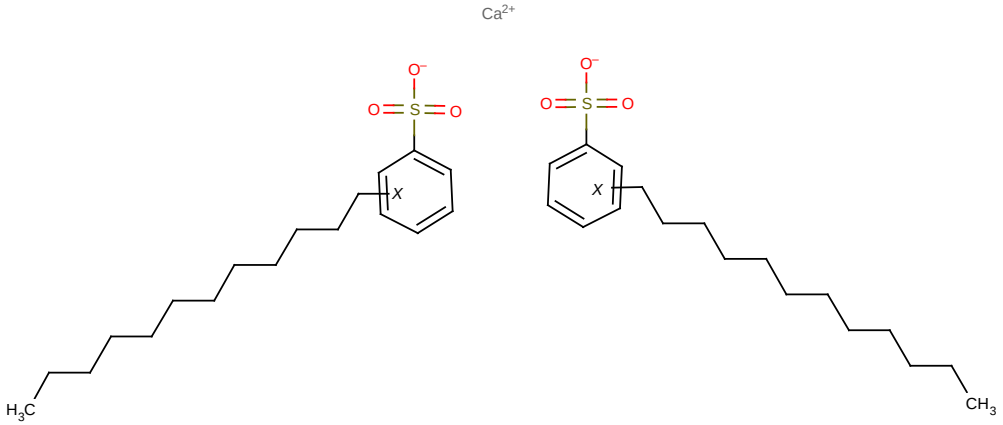
CAS RN: 27323-41-7 (linear)



Source – TOXNET, ECOSAR

Benzenesulfonic acid, dodecyl-, calcium salt

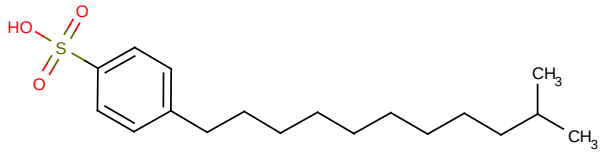
CAS RN: 26264-06-2 (linear)



Source – CHEMIDPLUS, ECOSAR

Benzenesulfonic acid, dodecyl-, branched

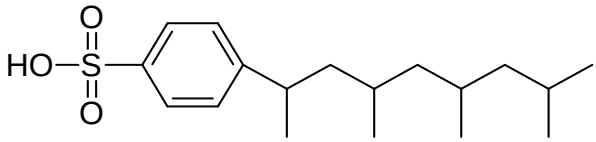
CAS RN: 68411-32-5 (branched)



Source – CHEMIDPLUS, ECOSAR

Benzenesulfonic acid, mono-C11-13-branched alkyl derivs.

CAS RN: 68608-88-8 (branched)

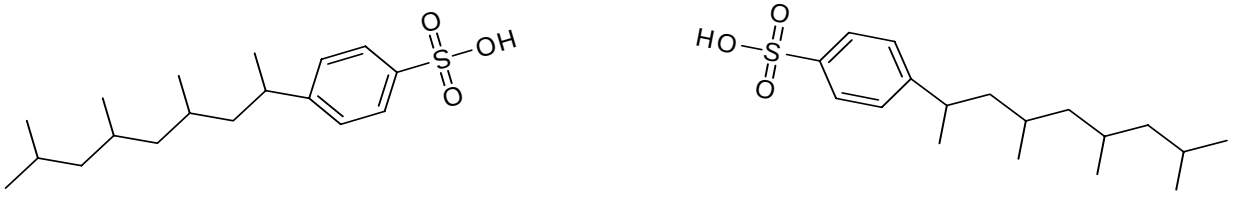


Source – ESIS, ECOSAR

Benzenesulfonic acid, mono-C11-13-branched alkyl derivs, calcium salts

CAS RN: 68953-96-8 (branched)

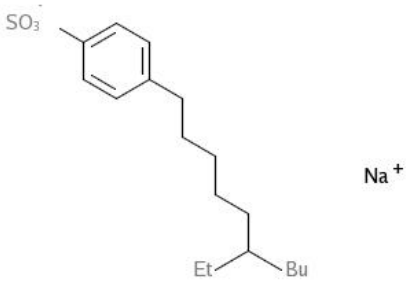
Ca 2^{+}



Source - ECOSAR

Benzenesulfonic acid, mono-C11-13-branched alkyl derivs, sodium salts

CAS RN: 68608-89-9 (branched)

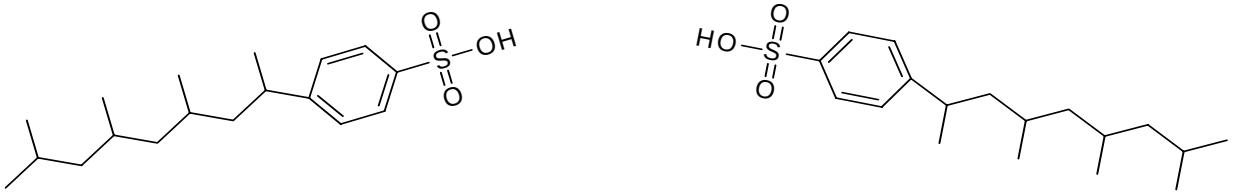


Source - ESIS

Benzenesulfonic acid, dodecyl-, branched, calcium salts

CAS RN: 70528-83-5 (branched)

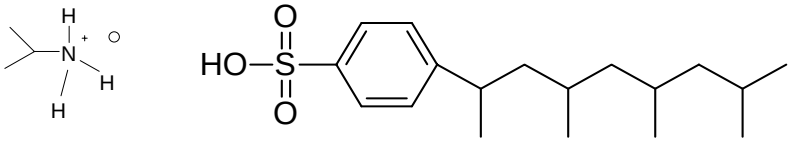
Ca 2+



Source - ECOSAR

Benzenesulfonic acid, dodecyl-, branched, compd. with 2-propanamine

CAS RN: 90218-35-2 (branched)



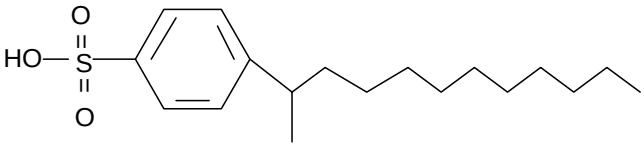
Source – ECOSAR

4.2 Supporting Chemicals

The four chemicals included as supporting chemicals for the LAS/ABS category are each depicted below. Each depiction includes the chemical name, the CAS RN, whether the chemical is a linear or branched structure, a representative drawing of the structure itself, and the source of the chemical structure. Two of the four supporting chemicals are representative chemicals from previous HPV Challenge submissions: benzenesulfonic acid, dodecyl (27176-87-0) is in the 2003 US HPV submission for LAB sulfonic acids; and sodium alkylbenzene sulfonate or benzenesulfonic acid, C10-13 alkyl derivs., sodium salt (68411-30-3) is in the 2005 OECD HPV submission for linear alkylbenzene sulfonates (LAS). Both of these previous submissions include multiple chemicals in their respective categories. The chemicals in the LAS category are anionic surfactants used in a wide range of industrial, commercial and consumer products. The LAB sulfonic acids are all used as intermediates in the production of LAS. For the purposes of this LAS/ABS submission, only a single, representative CAS RN is described for each of these two supporting categories, along with its corresponding HPV endpoint data. So in fact, the entire dataset for both of the categories could be used to support this LAS/ABS category submission.

Benzenesulfonic acid, alkyl deriv., linear

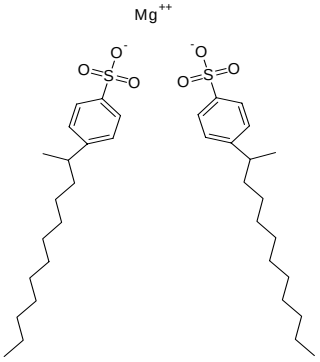
CAS RN: 42615-29-2 (linear)



Source – December 2002 submission

Benzenesulfonic acid, C10-16-alkyl derivs, magnesium salts

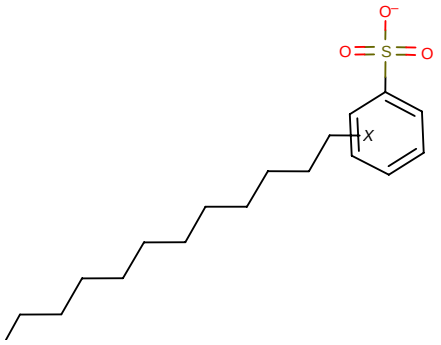
CAS RN: 68584-26-9 (linear)



Source - December 2002 submission

Benzenesulfonic acid, dodecyl

CAS RN: 27176-87-0 (linear)



Source – ECOSAR; Linear Alkylbenzene (LAB) Sulfonic Acid Category US HPV submission

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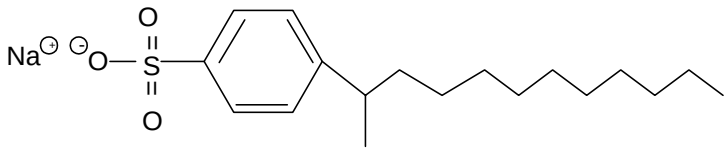
Sodium alkylbenzene sulfonate or Benzenesulfonic acid, C10-13 alkyl derivs., sodium salt

RN: 68411-30-3 (linear)



Source – ECOSAR; Linear Alkylbenzene Sulfonate (LAS) Category OECD HPV submission

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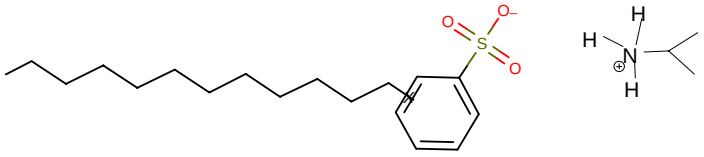
4.3 Synonymous chemicals

As stated above, because of nomenclature modifications adopted to provide more descriptive characterization of some of the LAS-ABS chemicals, three of the sponsored chemicals are identified by additional chemical names (commercial synonyms) and CAS RNs. Structures for the synonymous chemicals are provided below.

Benzenesulfonic acid, C10-16-alkyl derivs., compds. with 2-propanamine

CAS RN: 68584-24-7



SOURCE: representative structure drawn based on compound name

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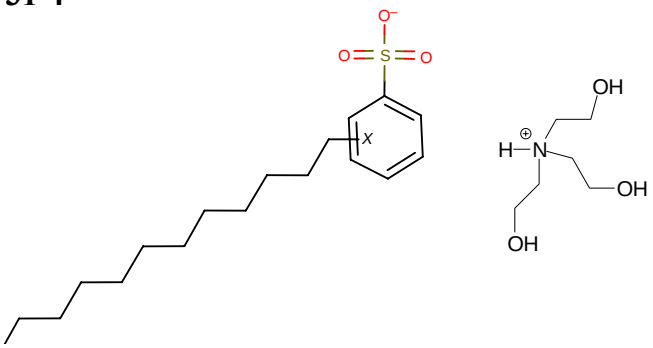
Benzenesulfonic acid, C10-13-alkyl derivs., compds. with Triethanolamine

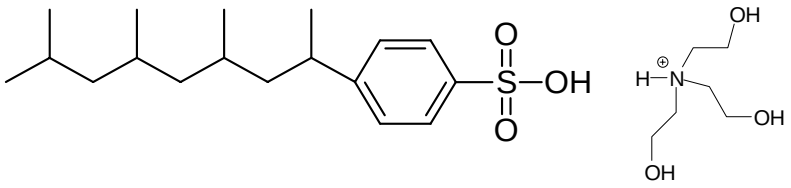
CAS RN: 68411-31-4



SOURCE: representative structure based on compound name

Benzenesulfonic acid, C10-13-alkyl derivs., compds. with triethanolamine

CAS RN: 70528-84-6



SOURCE: representative structure based on compound name

4.4 The LAS/ABS Chemicals as a Category

Chemical categories can be constructed on the basis of similar and/or patterned chemical structures and compositions as well as on similar and/or predictable physico-chemical, environmental fate and toxicological properties. As described previously, the nine sponsored chemicals (and sixteen total chemicals) found in this category are derived from comparable chemical reactions. The resulting structures are generally mixtures of C10 to C14 linear or mono-branched alkyl chains with a single benzene ring sulfonated at the *para* position attached (at various points) to the alkyl chain. Sponsored substances are either acid forms or they are salts (ammonium, calcium, or sodium). Supporting substances are either acid forms or they are salts (magnesium or sodium).

In water, all products of acid-base reactions at moderate to low concentrations are essentially completely dissociated into solvated ions at environmentally relevant pH levels. The sulfonic acids and their salts (other than ammonium) should dissociate almost completely up to the critical micelle concentration. At or above this point, any additional surfactant exists in micelle form and the counter ions are somewhat associated. The LAS/ABS surfactants will form micelles with an apolar core of alkyl tails and a surface consisting of sulfonate groups, thus rendering the surface negatively charged. The counter ions will be attracted by this negatively charged layer, thereby forming a now positively charged layer around the micelle (electronic double layer). Hence, semi-dissociation is observed for the LAS/ABS substances in aqueous solution above the critical micelle concentration. The substances with functionalized ammonium cations (26264-05-1, 27323-41-7, and 90218-35-2) are expected to remain intact in aqueous solutions.

The case for the nine sponsored chemicals to be considered a category on the basis of comparable/predictable physico-chemical, environmental fate and toxicological properties is made in the following pages that summarize these properties for the nine sponsored chemicals. The four supporting chemicals also share close chemical structure as well as fate and toxicological properties.

5 Summary of Endpoints

The available data are indicated in the following tables for each of the nine sponsored chemicals and for the four supporting chemicals. The corresponding number of the source reference is indicated in the column marked "Ref". The same source reference number appears in Section 7.2 *References for the robust summaries*.

Table 5.1 – physical/chemical endpoints
Table 5.2 – environmental fate endpoints
Table 5.3 – ecotoxicity endpoints
Table 5.4 – health effect endpoints

A descriptive summary for each of the endpoints is provided below. Beyond-SIDS data, to the extent they are available, are also included in both the tables and text.

When viewed as a whole, and considering the use and exposure characteristics of the nine sponsored chemicals, no additional testing is deemed necessary to characterize the SIDS

endpoints for the LAS/ABS category. There is considerable reliance on read-across for all but a couple endpoints, but the patterns point to the chemicals as having comparable and predictable physical/chemical properties, environmental fate as well as ecotoxicity and mammalian toxicity.

5.1 Physical-Chemical Endpoints

The physical-chemical properties of the LAS/ABS category affect partitioning between air and water and water and organic phases (i.e., soil, sediment and biota). The SIDS endpoints of vapour pressure, water solubility and partitioning coefficient are the main drivers. Because of the relatively narrow range of carbon chain lengths of chemicals in the category, it would be expected that their physical-chemical properties would be generally similar. The significance of linear versus branched alkyl chains can be seen in the available data which indicates that the property patterns are generally similar.

There are vapour pressure data for four of the chemicals including three linear and one branched structure (Table 5.1). Low vapour pressures for these four chemicals point to low volatility for the LAS/ABS category. This is further supported by the Mackay fugacity model prediction (Table 5.2) which indicates essentially 0% of these chemicals partitioning to air.

There are water solubility data/information for six chemicals including linear and branched structures indicating they are water soluble (Table 5.1). The acid and salt forms of the chemicals will be completely ionisable in water at environmentally relevant pH levels. Material safety data sheets carry the term “dispersible”, while structure activity models predict mg/L solubility and measurements are in the g/L solubility. Dispersible is an accurate descriptive term as surfactants form micelles in water. Again, the fugacity model prediction (Table 5.2) indicates about one quarter of the mass of any given chemical in this category would be in the water phase at equilibrium.

Octanol-water partition coefficient estimates range from about log 2 to log 7 (Table 5.1) using chemical structure activity relationships in several models including: the latest version of ECOSAR (v0.99h - 2007), as well as the QSAR method of Leo and Hansch (1979) as modified by Roberts (1991) for surfactant structures, and the Syracuse Research Corporation (SRC) PhysProp method (1995). The relatively large range of Kow values is inconsistent with the structural similarities across the category and between sponsored and supporting chemicals. In its 1996 review of LAS and related compounds, the IPCS noted that while the octanol-water partition coefficient can be calculated in practice, it is impossible to measure Kow for surface-active compounds like LAS.

Fugacity model predictions indicate about three-quarters of the mass of any given chemical in this category would be in the solid phase, either soils or sediments, at equilibrium (Table 5.2).

5.2 Environmental Fate Endpoints

Based on the vapour pressure it is unlikely that significant amounts of chemicals in the LAS/ABS category will be in the atmosphere. There is no evidence of photodegradation of these chemicals in water under environmental conditions and the absence of photolyzable groups suggests it is unlikely that this would be a significant mechanism for degradation. However,

photodegradation in water for a supporting chemical, CAS RN 68411-30-3, has been demonstrated in the presence of photoactivating materials. Greater than 95% photolytic degradation was measured in 20 minutes exposure to a 1200-watt mercury vapour lamp using ferric perchlorate as a sensitizer (Table 5.2).

Abiotic hydrolysis is not expected to degrade the chemicals in the LAS/ABS category. This is the conclusion of the single study reported for the supporting chemical, CAS RN 68411-30-3 (Table 5.2). The absence of readily hydrolyzable groups in the chemical structures of the category substances and the use pattern in shelf-stable liquid cleaning products supports that these chemicals should be stable in water.

Measured biodegradation data are available for two of the sponsored chemicals (including one linear and one branched structure) as well as for supporting chemicals (Table 5.2). Biodegradation is the primary mechanism by which the chemicals in the LAS/ABS category, as well as those in the supporting categories, are ultimately degraded in the environment. Biodegradation from 71-95% is reported for the sponsored linear structure CAS RN 27323-41-7. Using the OECD 301B protocol, the sponsored branched structure CAS RN 68411-32-5 degraded 64-73% after 28-days at 10 mg/L and 20 mg/L, respectively. This result meets the 10-day window for readily biodegradable at 10 mg/L but not at 20 mg/L. An extensive database of studies is available for the chemicals in the supporting LAS category, including biodegradation in the range of 76-94% in 28 days for CAS RN 68411-30-3, a linear C11-C13 structure (Table 5.2). These data are from four different test protocols including: the OECD 301A – DOC die away test, the OECD 301B – modified Sturm test, OECD 301E – ready biodegradability screening test, and OECD 303A – coupled unit test. In addition, there are two published reports of iso-branched LAS biodegradation. Both Cavalli et al. (1996) and Nielsen et al. (1997) report mineralization of the branched materials. The Nielsen study was performed using radiolabeled test material. While not included in Table 5.2, there are two additional biodegradation studies in the LAB Sulfonic Acid category submission that support the relatively rapid and complete biodegradation of the C10-C16 alkylbenzene sulfonate materials.

All of the studies and data reported above are for aerobic biodegradation. There are far fewer data on biodegradation under anaerobic conditions. Denger and Cook (1999) showed that strains of anaerobic bacteria isolated from wastewater treatment plants in Germany were capable of degrading LAS under anaerobic conditions in the laboratory when LAS was the sole source of sulphur. A more recent study (Lara-Martin et al., 2007) of LAS in anoxic marine sediments studied in the laboratory reported 79% degradation in 165 days and concluded that LAS may not be persistent in anoxic environments as previously thought.

No bioconcentration studies were identified for the sponsored chemicals in the LAS/ABS category; however, bioaccumulation has been reported for the supporting chemical benzenesulphonic acid, (C10-13) linear alkyl (Table 5.2). The study was performed using ^{14}C-ring-labeled LAS and the whole body bioconcentration factor (BCF) was measured at 104 following steady state which was reached after 7 days. The chemical was depurated rapidly once exposure was stopped. Based on these results, the chemicals in the LAS/ABS category are not expected to have significant bioaccumulation potential.

5.3 Ecotoxicity Endpoints

Ecotoxicity of the sponsored chemicals is assessed for SIDS endpoints using two approaches; acute toxicity measurements from studies with fish, invertebrates and algae, and toxicity predictions using quantitative structure activity relationships. Both are used to establish the patterns and trends in ecotoxicity that allow for read-across and thus an assessment for the entire category of sponsored chemicals.

Measurements

Acute fish toxicity data are available for two of the sponsored and three of the supporting chemicals. The measured LC50 values from 14 studies with eight fish species range from 1 to 20 mg/L (Table 5.3). The ECOSAR predicted LC50 value for the same five chemicals (all having effective alkyl chainlengths = 12) is 2.6 mg/L and range from 0.46 to 3.5 mg/L for the entire category. A range covering an order of magnitude or more is generally considered comparable for aquatic toxicity tests across a wide range of species and reported by different laboratories.

Acute daphnia toxicity data are available for the same two sponsored and two of the same three supporting chemicals. The measured LC50 values range from 2.2 to 15 mg/L for the five studies reported. ECOSAR predicts comparable toxicity for daphnia and fish for these chemicals (Table 5.3). Robust summaries are also provided for three additional aquatic invertebrates (the midge and two worms); the LC50 values are 1.8 to 6.5 mg/L which fall in the same range as for the daphnia and fish.

Algal toxicity is reported for one sponsored and two supporting chemicals. The EC50 values range from 5 to 300 mg/L for a total of eleven studies with two green algal species (Table 5.3). The ECOSAR predicted values are within the range of measured values; they are 96-hr EC50 values of 55-70 mg/L.

While not SIDS endpoints, there are robust summaries for six bacteria toxicity tests with one of the supporting chemicals. The measured EC50 values range from 60 to 350 mg/L. There are also robust summaries included for chronic toxicity for three fish species (a total of six studies) and for daphnia (two studies) for the same supporting chemical. The No Observed Effect Concentration (NOEC) values are all within an order of magnitude of each other (about 0.2 to 2.0 mg/L).

Finally, there are robust summaries for two additional beyond-SIDS endpoints, toxicity to terrestrial plants and terrestrial invertebrates. Studies for two of the supporting chemicals involving seven species of plants and two species of soil dwelling invertebrates (earthworms and springtails) indicate toxicity in the hundreds of parts per million (mg/kg) in soil.

Predictions

Representatives from the Consortium met with EPA OPPT experts in ECOSAR to obtain guidance on the proper use of the structure activity analysis for the LAS/ABS types of chemicals. The experts provided direction to find and use ECOSAR version 0.99h (2007) and also provided a printed table of predicted aquatic toxicity values (fish, daphnia and green algae) linked to the number of carbons (C2 – C22) in LAS-type anionic surfactants. The citation for the table is

"OPPT SAR for Anionic Surfactants". The ECOSAR predicted aquatic toxicity values for linear compounds in Table 5.3 are taken directly from the table provided by EPA. In order to predict aquatic toxicity values for branched compounds in the alkylbenzene sulfonate class, the effective chain length of each branched chemical had to be determined. This involves finding the closest match between the predicted log Kow of the branched alkyl portion of the chemical (using KOWWIN) and the predicted log Kow for a linear alkyl structure. This was accomplished in several steps. First, the SMILES notation of a given branched chemical was derived by entering its CAS RN into ECOSAR. Then the benzene ring and S-group were manually removed from SMILES leaving the alkyl chain. Next, the logKow prediction was determined for that "effective chain length". The predicted logKow value was matched to logKow values for linear alkyl chain compounds and that carbon chainlength was noted. Finally, that carbon chainlength was entered in ECOSAR under special class – anionic surfactant – alkyl benzene sulfonates and the model calculates corresponding aquatic toxicity values (96-hr LC50s) for fish, daphnia and algae. The EPA OPPT experts indicated that the algal toxicity values in the printed table they provided are a better approximation (than the ECOSAR generated value) for given carbon chainlengths. The toxicity values listed in Table 5.3 for the branched chemicals are ECOSAR predicted values for fish and daphnia and printed-table values for algae.

Example: 68953-96-8 benzenesulfonic acid, mono C11-13-branched alkyl derivs, sodium salts… The SMILES notation of the alkyl chain portion is c[c[c]cc[cc[cc[c]c]c]c]c; the KOWWIN estimated logKow for this structure is 6.92; which is equivalent to the logKow for a linear C13.5 LAS; the ECOSAR anionic surfactant – alkyl benzene sulfonate toxicity estimates for a C13.5 chainlength are: fish 96hr LC50 = 0.46 mg/L; daphnia 48-hr EC50 = 0.46 mg/L; and the printed-table value for algae 96-hr EC50 = 55 mg/L.

Sponsored and supporting chemicals are listed in Table 5.3 starting with the largest effective alkyl chainlengh at the top of the table and progressing to the smallest effective alkyl chainlength at the bottom of the table. The predicted acute aquatic toxicity decreases as the effective alkyl chainlength gets smaller.

5.4 Health Effect Endpoints

There are good reliability data for all of the SIDS endpoints (Table 5.4). However, read-across is needed for most of the endpoints. The acute oral toxicity data and the beyond-SIDS skin and eye irritation data establish a similar pattern of toxicity among the linear and branched chemicals in the LAS/ABS category.

The acute oral toxicity for three linear sponsored chemicals, three branched sponsored chemicals and for two supporting chemicals range from 520 mg/kg bw to 2320 mg/kg bw (or higher) (Table 5.4). The single reported acute dermal study for a sponsored chemical reported an LD50 of >4199 mg/kg bw. Rat and mouse subcutaneous dose studies for one of the supporting chemicals reported LD50 values ranging from 810 to 1400 mg/kg bw for males and females combined.

There is a single acute inhalation study reported for a supporting chemical (Table 5.4). The reported ALC value, defined as the lowest atmospheric concentration generated that caused death in one or more rats either on the day of exposure or within 14 days post exposure, is 310 mg/m^3 of

particulate. The robust summary points out however that the respirable size particles generated in the study (2.5 micron) are considerably smaller than those found in products in the marketplace. Direct extrapolation of the study results to human exposure and potential health effects is therefore not advised.

Genotoxicity data are available for two of the supporting chemicals (Table 5.4). Ames tests were negative for both chemicals. In addition, two *in vivo* tests, one conducted with Syrian hamster embryo cells and the other with mouse micronucleus cells, were also negative. These results support a conclusion that the chemicals in the category are not mutagenic.

A total of six repeat dose studies are reported for chemicals in the category; one for a sponsored chemical and the other five for two of the supporting chemicals (Table 5.4). The six studies cover a wide range of exposure routes and species including:, a 28-day simultaneous oral and subcutaneous exposure in monkeys, a 30-day gavage study in rats, a 90-day dermal study in rabbits, a 6-month drinking water study in mice, and 9-month diet and drinking water studies in mice. Two of the six studies (28-day monkey oral+sc and 90-day rabbit dermal) reported No Observable Adverse Effect Levels (NOAEL) above the doses administered, 60 mg/kg bw and 5 mg/kg bw, respectively. The 6-month mouse drinking water study reported liver cell effects at the single dose of 17 mg/kg bw. The 30-day rat gavage study reported a NOAEL of 125 mg/kg bw with effects at 250 mg/kg bw, and the 9-month mouse studies reported NOAELs of 250 and 500 mg/kg bw for drinking water and dietary exposures, respectively. The Lowest Observable Adverse Effect Levels (LOAEL) for these studies were 500 and 1000 mg/kg bw, respectively.

Three reproductive toxicity studies are reported for three of the chemicals in the category, one sponsored and two supporting (Table 5.4). They include two generation dermal and dietary exposure of rats, and exposure of fertilized mouse embryo cells.

- No treatment related effects were observed in pups over two generations following male rats being dosed on shaved skin for 10 weeks to 1.5 mg a.i./kg bw and then mated with untreated females. The NOAEL is therefore > 1.5 mg a.i./kg bw.
- Continuous dietary dosing of male and female rats at 103 and 222 mg a.i./kg bw, over two generations, was associated with slight retardation of somatic growth, but there were no adverse effects upon reproductive performance or fertility, thus the NOAEL for reproductive effects is >5000 mg/kg bw (>222 mg a.i /kg bw). The NOAEL based on growth of F2 pups up through lactation is 1250 mg/kg bw (=50 mg a.i./kg bw).
- Fertilized mouse embryo cells were exposed to a solution containing the test material over a range of concentrations for either one hour or continuously for five days. The NOAEL for blastocyst formation was 0.025% for a 1-hour exposure and 0.01% for a 5-day exposure.

Seven developmental toxicity studies are reported for the same sponsored and supporting chemicals evaluated for reproductive toxicity (Table 5.4). Exposures included three species (mouse, rat and rabbit) and both oral and dermal routes. The data indicate the chemicals in the category are not teratogenic or embryotoxic. Toxicity to the dams was observed in some of the studies and the NOAELs are consistent with those reported in the repeated dose studies.

- No treatment related effects were observed on fetuses following repeated exposure of female rats during 19 days of gestation to 10 mg/kg bw; NOAEL > 10 mg/kg bw.

- No teratogenic or embryopathic effects were observed when the dermis of pregnant rats was exposed for 20 straight days at concentrations that elicit marked skin changes and 5% reductions in maternal body weight. The NOAEL for developmental effects was > 400 mg/kg bw (= 82 mg a.i./kg bw).
- No teratogenic or embyrotoxic effects were observed following oral gavage of female rats, mice or rabbits exposed on days 6-18 of gestation to up to 600 mg/kg bw except in situations where there was marked toxicity to the dam. The NOAEL for developmental effects is >600 mg/kg bw. There were marked reductions in litter size following toxicity to the dam. NOAEL for maternal toxicity was > 2 but <300 mg/kg bw for mice and rabbits and 300 mg/kg for rats.
- No teratogenic or embyrotoxic effects were observed following dermal exposure of female rats, mice or rabbits exposed up to day 16 of gestation to up to 3% solution of test substance except in situations where there was marked toxicity to the dam. The NOAEL for developmental effects is >3% which is equivalent to >90, >60, >500 mg a.i./kg bw for rabbits, rats and mice, respectively. NOAEL for maternal toxicity was 0.3% = 50 mg/kg bw (mice), 0.3% = 9 mg/kg bw (rabbits) and 3% = 60 mg/kg bw (rats).
- No teratogenicity or embryotoxicity effects were observed following oral exposure of female rabbits from day 6 to 18 of gestation to as much as 250 mg/kg bw of the test substance; thus the NOAEL for developmental effects is >250 mg/kg bw. However, the NOAEL for maternal toxicity was 60 mg/kg bw based on post implantation loss.
- No teratogenicity, embryotoxicity or maternal toxicity was observed following topical application of up to 3% test solution to pregnant rabbits during days 6 to 18 of gestation. Clinical signs were observed but not considered toxicologically significant. The NOAEL is therefore >3%.
- No teratogenicity, embryotoxicity or maternal toxicity was observed following dermal application of up to 7% test solution to pregnant rats during days 7 to 17 of gestation. The NOAEL is therefore >7%.

There are also a number of reported studies for the beyond-SIDS endpoints of skin and eye irritation. They include results for three linear and three branched sponsored chemicals (Table 5.4). The results consistently show patterns of what amounts to "irritating to moderately irritating" to skin and "irritating to severely irritating" to eye. A single reported guinea pig sensitization test of 0.1% intracutaneous and 3% epidermal doses reports no sensitizing effects observed. Products containing the chemicals in the LAS/ABS category carry labels cautioning avoidance of exposure to skin and eyes.

Finally, the absorption, distribution, metabolism and elimination of LAS have been studied in several species, including rats, mice, guinea pigs, pigs and rhesus monkeys (Debane, 1978; Michael, 1968; Havermann and Menke, 1959; Cresswell et al., 1978; and Sunakawa et al., 1979). Robust summaries for these studies are provided in the OECD SIDS Initial Assessment Report for Linear Alkylbenzene Sulfonate (UNEP 2005). These studies are also cited in the WHO Environmental Health Criteria for Linear Alkylbenzene Sulfonates and Related Compounds (IPCS, 1996). Radiolabeled LAS was administered either topically (i.e., dermally) or orally. Results showed that LAS can be absorbed from the gastrointestinal tract. Absorbed LAS is then metabolized and excreted without accumulation in the major tissues or fat. The robust summary for a representative study with CAS RN 68411-30-3 (Michael, 1968) is included in the Appendix in Section 8.0.

Table 5.1 – Physical-Chemical Endpoints

	SPONSORED CHEMICALS								SUPPORTING CHEMICALS			
	Linear Structures						Branched Structures		Linear Structures			
Substance →	**26264-05-1**	*Ref*	**27323-41-7**	*Ref*	**26264-06-2**	*Ref*	**68953-96-8**	*Ref*	**68411-30-3**	*Ref*	**27176-87-0**	*Ref*
Melting point											-10 ºC	74
Boiling point	>149 ºC	22					117 ºC	3 & 4			205 ºC at 1013 hPa	74
Vapour pressure	<3100 Pa	22	ca. 8 x 10^{-27} Pa	71			733 Pa	3 & 4	3 x 10^{-13} Pa	43		
Partition coefficient (log Kow)	ca. log 6.18	83	ca. log 1.85	83 & 84	ca. log 6.78	83	ca. log 5.54	83	ca. log 3.32 ca. log 2.02	42 83	ca. log 1.96 ca. log 4.78	76 83
Water solubility	dispersible	22	ca. 27.1 mg/L	71	dispersible	21	dispersible	3 & 4	ca. 250 g/L	43	300 g/L	75

ca. – calculated; methods not specified for other values, therefore not know if measured or calculated

Table 5.2 - Environmental Fate Endpoints

Substance →	SPONSORED CHEMICALS										SUPPORTING CHEMICALS			
	Linear Structures				Branched Structures						Linear Structures			
	26264-05-1	*Ref*	**27323-41-7**	*Ref*	**68411-32-5**	*Ref*	**68608-88-8**	*Ref*	**68608-89-9**	*Ref*	**42615-29-2**	*Ref*	**68411-30-3**	*Ref*
Photodegradation													>95% in 20min	80
Hydrolysis													Stable in water	81
Distribution Between Environ. Comparts.													air = 0% water = 26% soil = 56% sediment = 18%	82
Biodegradation	biodegradable	40	71% in 28 days biodegradable 95%	20 41 37	64-73% in 28 days	25	biodegradable	38	biodegradable	39			76-94% in 28 days	44 - 51
Bioconcentration											BCF = 104	8	104	8

Table 5.3 - Ecotoxicity Endpoints

Substance	Type	Chemical Name	Effective alkyl chain length	Predicted Toxicity for Anionic Surfactants (mg/L)		Measured Acute Toxicity (mg/L)		Predicted Toxicity for Anionic Surfactants	Measured Acute Toxicity (mg/L)
				Fish 96hr LC50	Daphnia 48hr EC50	Fish 96hr LC50	Daphnia 48hr EC50	Algae 96hr EC50	Algae 96hr EC50
68608-89-9	SP	Benzenesulfonic acid, mono-C11-13-**branched** alkyl derivs, sodium salts	C13.5	0.46	0.46			55	
68953-96-8	SP	Benzenesulfonic acid, mono-C11-13 -**branched** alkyl derivs., calcium salts	C13.5	0.46	0.46			55	
68584-26-9	SU	Benzenesulfonic acid, C10-16- alkyl derivs., magnesium salt	C13	0.75	0.75				
70528-83-5	SP	Benzenesulfonic acid, dodecyl-, **branched**, calcium salts	C12.5	1.3	1.3				
42615-29-2	SU	Benzenesulfonic acid, linear alkyl	C12	2.6	2.6	3.4 - 4.0[d]		70	
26264-06-2	SP	Benzenesulfonic acid, dodecyl-, calcium salt	C12	2.6	2.6				
27323-41-7	SP	Benzenesulfonic acid, dodecyl-, compd. with 2,2',2"-nitrilotris[ethanol]	C12	2.6	2.6	1 - 5[e]	15.0[e]	70	11 - 300[e]
26264-05-1	SP	benzenesulfonic acid, dodecyl-, compd. with 2-propanamine (1:1)	C12	2.6	2.6	20.0[f]	2.2[g]	70	
27176-87-0	SU	Benzenesulfonic acid, dodecyl	C12	2.6	2.6	4.1[h] & 4.3[i]	5.88[j] &12[h]	70	29[j]
68411-30-3	SU	benzenesulfonic acid, C10-13 alkyl derivs., sodium salt	C12	2.6	2.6	2.2 - 7.8[a]	1.62 – 9.3[b]	70	5 - 163[c]
68411-32-5	SP	Benzenesulfonic acid, dodecyl-, **branched**	C11.9	2.9	2.9				
68608-88-8	SP	Benzenesulfonic acid, mono-C11-13 -**branched** alkyl derivs.	C11.8	3.5	3.5				
90218-35-2	SP	Benzenesulfonic acid, dodecyl-, **branched**, compds with 2-propanamine	C11.8	3.5	3.5				

Table legend – Chemicals are ordered from top to bottom to reflect largest to smallest effective alkyl chainlength. Predicted toxicity values are from EPA structure activity models (ECOSAR v0.99h). “Type” refers to sponsored chemical (SP) and supporting chemical (SU). Sources of measured values are indicated by superscript following the data entry; i.e., “a” is references 42, 47 and 52 -55, “b” is references 42, 43 and 52, “c” is references 42, 43, 47, 52, 56-58 ,“d” is reference 14 , “e” is 37, “f” is reference 10, “g” is reference 24, “h” is reference 77, “i” is reference 78, “j” is reference 79

Table 5.4 - Human Health Endpoints

Substance →	SPONSORED CHEMICALS										SUPPORTING CHEMICALS			
	Linear Structures						Branched Structures				Linear Structures			
	26264-05-1	*Ref*	27323-41-7	*Ref*	26264-06-2	*Ref*	68411-32-5	*Ref*	68608-88-8	*Ref*	90218-35-2	*Ref*	42615-29-2	*Ref*	68584-26-9	*Ref*	68411-30-3
Acute oral	1836 mg/kg 1300 mg/kg	22 32	1653 mg/kg >1953 mg/kg 2320 mg/kg bw	9 1 37	1300 mg/kg	21	1080 mg/kg	15	520 mg/kg	17	1.8 mL/kg	36	650 mg/kg	17			1080 -1630 mg/kg Refs 60 - 63
Acute dermal			>4199 mg/kg	1													810-1250 mg/kg (subcutaneous) Ref 63
Acute inhalation																	310 mg/m^3 Ref 72
Genotoxicity (*in-vivo*)													Negative in SHE-cells	6			Negative in mouse micronucleus assay Ref 73
Genotoxicity (*in-vitro*)													Negative in Ames	6			Negative in Ames Ref 70
Repeat Dose Toxicity			Rabbit 90-day dermal NOAEL >5 mg/kg bw (only dose tested)	1									Monkey 28-day oral + subcutan. NOAEL > 60 mg/kg bw Mouse 6- mo. drinking water NOAEL < 17 mg/kg (single dose)	5 30			Rat 30-day gavage NOAEL 125 mg/kg bw Refs 63 & 68 Mouse 9-mo NOAELs 250 mg/kg bw in drinking water, 500 mg/kg bw in diet Refs 42, 68, 69

Substance →	SPONSORED CHEMICALS									SUPPORTING CHEMICALS					
	Linear Structures						Branched Structures						Linear Structures		
	26264-05-1	*Ref*	27323-41-7	*Ref*	26264-06-2	*Ref*	68411-32-5	*Ref*	68608-88-8	*Ref*	90218-35-2	*Ref*	42615-29-2	*Ref*	68584-26-9	*Ref*	68411-30-3
Reproduc-tion /			Rat 2-gen. dermal NOAEL >1.5 mg/kg bw (only dose tested)	1									Mouse embryo incubate NOAEL 0.025% for 1-hr 0.01% for 5-day	7	Rat 2 gen. dietary NOAEL repro = 5000 (222 a.i.); F2 growth = 1250 (50 a.i.) mg/kg bw	29	
Develop-mental			Rat dermal teratox NOAEL F0 & F1 >10 mg/kg bw (only dose)	1									Rat dermal teratox NOAEL > 82 mg ai /kg bw	2	Rabbit oral teratox NOAEL >250 mg/kg bw; Maternal tox NOAEL = 60 mg/kg bw	26	
													3 sp. oral teratox NOAEL > 600 mg/kg bw for 3 species. Maternal tox NOAEL rat = 300, rabbit >2<300, mouse >2<300 mg/kg bw	18	Rabbit dermal teratox NOAEL - F0 & F1 >3% (max. dose)	27	
													3 sp. dermal Teratox NOAEL > 60, 90, 500 mg a.i./kg bw for 3 species. Maternal tox NOAEL rat = 60, rabbit = 9, mouse =50 mg/kg bw	19	Rat dermal teratox NOAEL - F0 & F1 >7% (max. dose)	28	

Substance →	SPONSORED CHEMICALS										SUPPORTING CHEMICALS		
	Linear Structures						Branched Structures				Linear Structures		
	26264-05-1	*Ref*	27323-41-7	*Ref*	26264-06-2	*Ref*	68411-32-5	*Ref*	68608-88-8	*Ref*	90218-35-2	*Ref*	42615-29-2	*Ref*	68584-26-9	*Ref*	68411-30-3
Irritation																	
• skin	Irritating	31	Irritating	11	Moderately Irritating	21	Irritating	11	Irritating	13	Moderately Irritating	35					Irritating Ref 64
			Irritating	37					Irritating	12	Non Corrosive	33					
• eye	Irritating	23			Severely Irritating	21					Highly Irritating	34					Irritating Refs 65 - 66
sensitization																	Not Sensitizing Ref 67

6 Ecological and Human Health Assessment

Detailed ecological and human health assessments have been published for linear alkylbenzene sulfonates as part of the OECD High Production Volume Chemicals Program. These reports include the SIDS Initial Assessment Report of LAS (UNEP 2005 and CLER 2005) and the Human and Environmental Risk Assessment (HERA) of LAS (CLER 2004). The Council for LAB/LAS Environmental Research (CLER) continues to assemble and report new studies and update the assessment findings; the most recent being the CLER REVIEW (2007).

The USA (EPA) was the sponsor country for the OECD SIDS Initial Assessment of LAS. The conclusions in the SIDS initial assessment profile for the LAS category (UNEP 2005) are: 1) the chemicals in the LAS category are currently of low priority for further work because of their low [human health] hazard potential except for skin and eye irritation and acute inhalation. Other countries may desire to investigate any exposure scenarios that were not presented by the Sponsor Country; and 2) the chemicals in the LAS category possess properties indicating a hazard for the environment (fish, invertebrates and algae). However, they are of low priority for further work due to ready and/or rapid biodegradation and limited potential for bioaccumulation.

The human and ecological exposures and risk assessments detailed in the UNEP and CLER documents are based on current LAS volumes, concentrations by product type, and product uses. On the human side, occupational exposure scenarios include workers in production and manufacturing where facility and equipment design practices and personal protective equipment limit exposure. Quantitative risk assessments were performed for a number of human exposure scenarios including: drinking water and fish consumption following environmental release; dermal exposure, and incidental and accidental ingestion and inhalation from a wide range of consumer product uses. Labelling of consumer products containing LAS and other surfactants include warnings of the potential for eye irritation as well as first aid instructions. On the ecological side, quantitative risk assessments were performed for representative manufacturing facility releases to the aquatic environment and for consumer product down-the-drain releases to wastewater treatment facilities that discharge treated effluent to the aquatic environment. Both monitoring and modeling information were used to predict human and ecological risks.

In lieu of quantitative exposure and initial risk assessments for the LAS/ABS category, a comparative evaluation is provided below by direct reference to the detailed assessments for the LAS category (UNEP, 2005; CLER 2005). The conclusion of such a comparison is that the LAS category can be extrapolated to the LAS/ABS category with rough equivalency for human exposures and risks whereas the aquatic exposures and risks would be proportionately smaller, based on a 98+% smaller down-the-drain volume of LAS/ABS category chemicals; more supporting details follow.

The chemicals in this LAS/ABS category generally have similar uses in industrial, commercial and consumer product uses as do the chemicals in the LAS category; that is, they are anionic surfactants. Chemical concentrations are generally the same for comparable uses. The industrial/commercial products typically contain >50% of the anionic surfactant and consumer products typically contain <30% of the anionic surfactant. The OECD SIDS for the LAS category (UNEP 2005) reports 390,000 metric tonnes produced/used annually in the US (2000).

That is equivalent to about 860,000,000 pounds/year. The chemicals in the LAS/ABS category are produced/used at about 21,000,000 pounds/year or roughly 2.5% of the volume of the much larger LAS category. The 21,000,000 pounds includes about 5,000,000 pounds used as intermediates in the production of LAS and about 12,000,000 pounds used in industrial/commercial products. The balance, about 4,000,000 pounds, is used in consumer products. Human exposure to the LAS/ABS category of chemicals would be generally comparable in industrial, commercial and consumer products. Therefore, the exposure and risk assessments for the LAS category can be used as reasonable surrogate estimates for the LAS/ABS category. On the ecological side, the difference between 16,000,000 pounds in industrial, commercial and consumer products for the LAS/ABS category and 860,000,000 pounds per year for the LAS category equates to <2% in the amount of chemical going down-the-drain, being treated and the residual being released to surface waters. Predicted ecological exposures and risks would therefore be proportionately smaller (98+% smaller) for the LAS/ABS category.

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[Note: Only the first 32 were included in the Dec 2002 submission]

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